

The similarity of attractive and repulsive forces on a lattice

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Abstract

On a lattice, as the momentum space is compact, the kinetic energy is bounded not only from below but also from above. It is shown that this, somehow removes the distinction between repulsive and attractive forces. In particular, it is seen that a region with attractive force would appear forbidden for states with energies higher than a certain value, while repulsive forces could develop bound-states. An explicit transformation is introduced which transforms the spectrum of a system corresponding to a repulsive force, to that of a similar system corresponding to an attractive force. Explicit numerical examples are presented for discrete energies of bound-states of a particle experiencing repulsive force by a piecewise constant potential. Finally, the parameters of a specific one dimensional translationally invariant system on continuum are tuned so that the energy of the system resembles the kinetic energy of a system on a one dimensional lattice. In particular, it is shown that the parameters could be tuned so that while the width of the first energy band and its position are kept finite, the energy gap between the first energy band and the next energy band go to infinity, so that effectively only the first energy band is relevant.

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1 Introduction

Formulation of physics on lattices has a distinguished place in many areas of physics, from condensed matter physics to high energy physics. In condensed matter physics, lattice formulations are mainly used as an approximation to the real model, which is on the continuum. For example as a crystal is symmetric under discrete translations, to study the motion of a particle one could use a simple lattice model (rather than the continuum) which has the same symmetries. Such a simplified model does lead to a band structure for the energy spectrum, although it results in only a single band, [1].

In high energy physics, there are cases where lattices are used as approximations of continuum, examples of which are lattice field theories and specially lattice gauge theories as numerical approximations for the original theories on continuum [2,3]. There are, however, models which regard the space to be fundamentally discrete. Examples are theories formulated on noncommutative spaces of Lie type noncommutativity, where the underlying Lie group is compact [4,5].

A remarkable feature of mechanics on a lattice is that the corresponding momentum space is compact. So for a particle on a lattice, any continuous function of the momentum, including kinetic energy, would be bounded both from below and above.

The purpose of the present work is to explore the consequences of the above-mentioned feature. In particular, it is shown that as a result of the kinetic energy being bound from both below and above, the distinction between repulsive and attractive forces is somehow blurred. As a result, a region with positive kinetic energy, which is supposed to be allowed would be forbidden if the energy is so high that the kinetic energy exceeds its upper bound. Similarly, systems with repulsive forces could develop bound-states. As will be seen, there is in fact a one-to-one correspondence between the spectrum (bounded or unbounded) of a system with a certain potential energy, and that of another system with a potential energy minus that of the former.

To have a taste of the exact statement, let us consider the cases when potential at infinity, $U(\infty)$, is larger (smaller) than the potential at finite distances, corresponding to attractive (repulsive) forces. For a particle on a continuum, the total energy cannot be everywhere smaller than the potential energy. Hence for repulsive forces the energy is larger than $U(\infty)$, meaning that far distances are in classically allowed regions, and the system is unbounded. Furthermore, there is no constraint on the energy levels, except that they should be larger than $U(\infty)$. Hence the energy levels are unbounded from above. For attractive forces, there could be energy levels which are smaller than $U(\infty)$. These correspond to bound-states, where far distances are in the classically forbidden region.

On a lattice, however, the kinetic energy is bounded from both below and above. That results in the classically forbidden region to consist of points where the kinetic energy is either less than its lower bound (K_{\min}), or larger than its upper bound (K_{\max}). Hence, the energy cannot be everywhere smaller than the potential energy plus K_{\min} or larger than the potential energy plus K_{\max} . An

energy level which is larger than $U(\infty) + K_{\max}$, corresponds to a bound-state. So repulsive forces could result in bound states as well. Also, for attractive forces, there is no energy level larger than $U(\infty) + K_{\max}$.

The scheme of the paper is the following. In section 2, the relation of the position space being discrete (lattice) with the momentum space being compact is investigated, with particular attention on the kinetic energy as a continuous function of the momentum space. In section 3, a system is studied which consists of a particle on a one dimensional lattice, experiencing a position dependent potential energy. The corresponding eigenvalue problem is discussed, including the relation between the spectrums corresponding to attractive and repulsive forces, and a particular example is studied in detail, to find the number and values of the bound energy levels. In section 4, a toy model is presented in which a particle moves on continuum under the influence of a periodic potential energy. The model is a Kronig-Penney type [6], consisting a particle moving in a periodic array of Dirac delta potential energies. It is shown that the parameters of the model could be tuned so that of the width and position the first energy band is kept fixed, while the gap between the first band and the next band tend to infinity. The first band could then be regarded as the values of the kinetic energy for a particle moving on a lattice. So a system on the continuum could be effectively changed to a system on a lattice.

2 Lattice and the compact momentum space

Consider a one dimensional infinite lattice. The Hilbert space for a particle living on such a lattice is spanned by the set of orthonormal kets $|n\rangle$ (with n being integer):

$$\langle n|n'\rangle = \delta_{nn'}. \quad (1)$$

So $|\psi\rangle$, the state vector of the particle can be represented by the wave-function ψ with

$$\psi(n) = \langle n|\psi\rangle. \quad (2)$$

Alternatively, one can use the Fourier-transformed basis, the set of the orthonormal kets $|s\rangle$:

$$|s\rangle = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} \exp(-i n s) |n\rangle. \quad (3)$$

$$|n\rangle = \int_{-\pi}^{\pi} \frac{ds}{\sqrt{2\pi}} \exp(i n s) |s\rangle. \quad (4)$$

It is seen that

$$\langle s|s'\rangle = \delta_p(s - s'), \quad (5)$$

where δ_p is the periodic Dirac delta:

$$\delta_p(s) = \sum_{j=-\infty}^{\infty} \delta(s - 2\pi j). \quad (6)$$

The Kinetic energy K would be a function of the lattice translation T with

$$T |n\rangle = |n+1\rangle. \quad (7)$$

It is seen directly from (3) that $|s\rangle$ is an eigenket of T :

$$T |s\rangle = \exp(i s) |s\rangle. \quad (8)$$

As the kinetic energy is a function of T , the ket $|s\rangle$ should be an eigenket of K as well:

$$K |s\rangle = \tilde{K}(s) |s\rangle, \quad (9)$$

where $\tilde{K}(s)$ is the corresponding eigenvalue. As

$$|s+2\pi\rangle = |s\rangle, \quad (10)$$

the set of the values of s resulting in distinct kets $|s\rangle$ is compact (the momentum space is compact). Hence (assuming that the function \tilde{K} is continuous), the set of the eigenvalues of the kinetic energy is also compact, namely it has a minimum K_{\min} and a maximum K_{\max} . The function \tilde{K} should also be periodic (with the period 2π) in s . In the case of free particle, for which the Hamiltonian H has only the kinetic part, the energy is bounded from both below (similar to the case of a free particle on continuum) and above.

A simple choice for the Kinetic energy is

$$\tilde{K}(s) = K_0 (1 - \cos s). \quad (11)$$

This is periodic, behaves like s^2 for small values of s , and is increasing with $|s|$ as long as s is in $[-\pi, \pi]$. One can express the constant K_0 in terms of the dimensional parameters m (the mass of the particle) and ℓ (the lattice spacing):

$$K_0 = \frac{\hbar^2}{m \ell^2}. \quad (12)$$

For the simple choice (11), one has

$$\begin{aligned} K &= \frac{K_0}{2} (2 - T - T^{-1}), \\ &= -\frac{K_0}{2} D^2, \end{aligned} \quad (13)$$

where D^2 is the Laplacian on the lattice:

$$(D^2 \psi)(n) = \psi(n+1) + \psi(n-1) - 2\psi(n). \quad (14)$$

Obviously, for the kinetic energy of the form (11),

$$\begin{aligned} K_{\min} &= 0. \\ K_{\max} &= 2 K_0. \end{aligned} \quad (15)$$

3 Position-dependent forces

Similar to the case of a particle moving on a one dimensional (continuous line), the Hamiltonian H of a particle moving influenced by a position-dependent force on a lattice, is the sum of the kinetic energy and the potential energy U ,

$$H = K + U, \quad (16)$$

where U is a function of the lattice site. That is, $|n\rangle$ is an eigenket of U with the eigenvalue $U(n)$:

$$U |n\rangle = U(n) |n\rangle. \quad (17)$$

Corresponding to any eigenvalue E of the Hamiltonian H , the (classically) forbidden region is defined as the set of points n for which

$$[E - U(n)] \notin [K_{\min}, K_{\max}]. \quad (18)$$

As the eigenvalues of the kinetic energy belong to the set $[K_{\min}, K_{\max}]$, the expectation value of $(K - K_{\min})(K_{\max} - K)$ is nonnegative. That is, for any ket $|\psi\rangle$,

$$\langle\psi| (K - K_{\min})(K_{\max} - K) |\psi\rangle \geq 0. \quad (19)$$

So,

$$\langle\psi| (H - U - K_{\min})(K_{\max} - H + U) |\psi\rangle \geq 0. \quad (20)$$

This is true if $|\psi\rangle$ is an eigenket of H with corresponding to the eigenvalue E as well. In that case, one arrives at

$$\langle\psi| (E - U - K_{\min})(K_{\max} - E + U) |\psi\rangle \geq 0, \quad (21)$$

or

$$\sum_n [E - U(n) - K_{\min}] [K_{\max} - E + U(n)] |\psi(n)|^2 \geq 0. \quad (22)$$

The multiplier of $|\psi(n)|^2$ in the above is negative, if n belongs to the forbidden region. This shows that the Hamiltonian has no eigenvalue for which everywhere is in the forbidden region. This is a generalization of the statement for the continuum, that there Hamiltonian has no eigenvalue which is less than the minimum of the potential energy (if such a minimum exists).

3.1 Relation between attractive and repulsive forces

Consider a Hamiltonian of the form (16). Let us restrict to the case that the kinetic energy has the following property

$$\tilde{K}(s + \pi) + \tilde{K}(s) = K_{\max} - K_{\min}. \quad (23)$$

This is obviously satisfied by the simple choice (11). In fact it mean that \tilde{K} is a constant plus an odd function of $\exp(is)$. Defining H' similarly but with $(-U)$ instead of U , it is seen that

$$\begin{aligned} H' &= K - U, \\ &= -[(K_{\max} - K_{\min} - K) + U] + (K_{\max} - K_{\min}). \end{aligned} \quad (24)$$

Defining the unitary operator S through

$$S |n\rangle := \exp(i\pi n) |n\rangle, \quad (25)$$

it is seen that

$$\{S, T\} = 0, \quad (26)$$

hence

$$S K S^{-1} = K_{\max} - K_{\min} - K. \quad (27)$$

It is also seen that

$$[S, U] = 0. \quad (28)$$

So,

$$H' = -S H S^{-1} + K_{\max} - K_{\min}. \quad (29)$$

This shows that the eigenvalues and eigen-functions of H' have a simple relation to those of H , namely if

$$H |\psi\rangle = E |\psi\rangle, \quad (30)$$

then

$$H' |\psi'\rangle = E' |\psi'\rangle, \quad (31)$$

(and, of course, vice versa) where

$$|\psi'\rangle = S |\psi\rangle. \quad (32)$$

$$E' = -E + K_{\max} - K_{\min}. \quad (33)$$

One has

$$\psi'(n) = \exp(i\pi n) \psi(n). \quad (34)$$

If U corresponds to a so called attractive force, then $(-U)$ corresponds to a repulsive force. But the spectrum of H' is similar to that of H . Especially, if the eigenvector $|\psi\rangle$ of H is a bound-state, that is the corresponding wave-function decays exponentially when its argument tends to $\pm\infty$, then so is the corresponding eigenvector $|\psi'\rangle$ of H' . Here, repulsive forces do give rise to bound-states as well, in contrast to what happens in continuum. But the bound-states corresponding to the repulsive forces occur for high energies, rather than low energies, where the bound-states corresponding to attractive forces occur.

3.2 Piecewise constant potential energies

When the potential energy is a piecewise constant function of the (discrete) position, the eigenket of the Hamiltonian is found similar to the case of the continuum, namely, one takes the eigenket ψ to be piecewise a linear combination of plane waves. In each region (where the potential energy is constant) the wave number is real if the region is not in the forbidden region. Otherwise, the wave numbers are complex. To solve the eigenvalue problem, one should write the continuity equation at boundaries.

For definiteness, for now on it is assumed that the kinetic energy is of the form (11). Then in each region, the eigenket ψ is a linear combination of two plane waves. At each boundary, one writes a continuity condition and the eigenvalue equation corresponding to that point. So if there are q regions, one has $2(q-1)$ equations between the coefficients of the wave-function. In each of the two regions which extend to $-\infty$ and $+\infty$, if the wave number is not real the boundary condition that the wave-function does not blow up at infinity makes the coefficient of one of the plane waves vanish. So there are $2q$ coefficients of the plane waves, if neither of the regions extending to infinity are forbidden, $(2q-1)$ coefficients of the plane waves, if one and only one of the regions extending to infinity are forbidden, and $(2q-2)$ coefficients of the plane waves, if both of the regions extending to infinity are forbidden. Then, similar to the case of the continuum, the spectrum of the Hamiltonian is continuous and the eigenspace is two-dimensional if neither of the regions extending to infinity is forbidden, the spectrum of the Hamiltonian is continuous and the eigenspace is one-dimensional if one and only one of the regions extending to infinity is forbidden, and the spectrum of the Hamiltonian is discrete if both of the regions extending to infinity are forbidden. The difference with the case of the continuum is that here the forbidden region is where the energy is either smaller than the potential energy or larger than the potential energy plus $2K_0$.

An example of a piecewise constant potential energy is

$$U(n) = \begin{cases} +\infty, & n \leq 0 \\ U_I, & 0 < n \leq n_0 \\ U_{II}, & n > n_0 \end{cases} \quad (35)$$

The energy eigenket ψ corresponding to such a potential energy is found in a way similar to the case of continuous space, namely

$$\psi(n) = \begin{cases} 0, & n \leq 0 \\ \psi_I, & 0 < n \leq n_0 \\ \psi_{II}, & n > n_0 \end{cases} \quad (36)$$

Denoting the regions $0 < n < n_0$ and $n > n_0$ with I and II, respectively, it is seen that the eigenvalue equation in these regions would be

$$(E - U_a) \psi_a = -\frac{K_0}{2} D^2 \psi_a, \quad (37)$$

where a is either I or II. The solution to (37) is

$$\psi_a(n) = A_a \exp(i s_a n) + B_a \exp(-i s_a n), \quad (38)$$

with A_a and B_a being constants, and s_a determined through

$$E - U_a = K_0 (1 - \cos s_a). \quad (39)$$

The boundary condition at $n = 0$ reads

$$A_I + B_I = 0, \quad (40)$$

so that

$$\psi_I(n) = A \sin(s_I n). \quad (41)$$

The boundary conditions at $n = n_0$ are

$$A \sin(s_I n_0) = A_{II} \exp(i s_{II} n_0) + B_{II} \exp(-i s_{II} n_0). \quad (42)$$

$$A \sin[s_I (n_0 + 1)] = A_{II} \exp[i s_{II} (n_0 + 1)] + B_{II} \exp[-i s_{II} (n_0 + 1)]. \quad (43)$$

If the region II is forbidden, of A_{II} and B_{II} the coefficient corresponding to a negative imaginary part for the wave number should vanish. Choosing by convention that the imaginary part of s_{II} be nonnegative, it is seen that in that case B_{II} is vanishing, so that the boundary conditions at $n = n_0$ become

$$A \sin(s_I n_0) = A_{II} \exp(i s_{II} n_0). \quad (44)$$

$$A \sin[s_I (n_0 + 1)] = A_{II} \exp[i s_{II} (n_0 + 1)]. \quad (45)$$

The condition that these equations have nontrivial solutions for A and A_{II} is then

$$\sin[s_I (n_0 + 1)] = \exp(i s_{II}) \sin(s_I n_0). \quad (46)$$

If the region II is forbidden, the wave-function decays exponentially in that region. Such wave-functions correspond to bound-states. One notes that the region II is forbidden, either if the energy is less than some value (U_{II}), or when it is larger than some value ($U_{II} + 2K_0$), unlike the case of continuum that bound-states occur only if the energy is less than a certain value. It is also seen that if K_0 tends to infinity (which corresponds to $\ell \rightarrow 0$, the continuum), the new possibility for bound-states is lost and one recovers the continuum results. One also notes that of the two possibilities resulting in the region II being forbidden, only one can be realized. The reason is that the whole lattice cannot be forbidden. If U_I is smaller than U_{II} , the so called potential well, then the only way that the region II be forbidden is that E be smaller than U_{II} . If U_I is larger than U_{II} , the so called potential barrier, then the only way that the region II be forbidden is that E be larger than $(U_{II} + 2K_0)$.

A shift in the potential energy is equivalent to a shift in the energy. So without loss of generality one can put

$$U_{II} = 0. \quad (47)$$

There remains then, only U_I . It is denoted by $\pm U_0$, where U_0 is positive. The minus (plus) sign, then corresponds to a potential well (barrier).

3.3 The potential well

There are two possible regions for the energy:

$$\begin{cases} \text{continuous spectrum,} & 0 \leq E \leq 2K_0 \\ \text{discrete spectrum,} & -U_0 < E < \min(0, 2K_0 - U_0) \end{cases} \quad (48)$$

For the discrete case, the energies are determined through (46). One has

$$s_{\text{II}} = i \cosh^{-1} \left(1 - \frac{E}{K_0} \right). \quad (49)$$

$$s_{\text{I}} = \cos^{-1} \left(1 - \frac{E + U_0}{K_0} \right). \quad (50)$$

If

$$U_0 > 2 K_0, \quad (51)$$

then there is a gap between the band of continuous spectrum, and the possible band of the discrete spectrum.

3.4 The potential barrier

There are two possible regions for the energy:

$$\begin{cases} \text{continuous spectrum,} & 0 \leq E \leq 2 K_0 \\ \text{discrete spectrum,} & \max(2 K_0, U_0) < E < 2 K_0 + U_0 \end{cases}. \quad (52)$$

For the discrete case, the energies are determined through (46). One has

$$s_{\text{II}} = \pi + i \cosh^{-1} \left(\frac{E}{K_0} - 1 \right). \quad (53)$$

$$s_{\text{I}} = \cos^{-1} \left(1 - \frac{E - U_0}{K_0} \right). \quad (54)$$

Again, there is a gap between the band of continuous spectrum, and the possible band of the discrete spectrum, if (51) is satisfied.

The number of the discrete energies can be studied as follows. Changing U_0 , while other quantities are kept constant, results in a change of the discrete energies and their corresponding eigenvectors. However, the derivative of the energies with respect to U_0 does not contain the derivative of the eigenvector:

$$\begin{aligned} \frac{dE}{dU_0} &= \frac{d\langle \psi | H | \psi \rangle}{dU_0}, \\ &= \left\langle \psi \left| \frac{dH}{dU_0} \right| \psi \right\rangle, \\ &= \sum_{n=1}^{n_0} \langle \psi | n \rangle \langle n | \psi \rangle, \end{aligned} \quad (55)$$

where $|\psi\rangle$ is the normalized eigenvector of H corresponding to the eigenvalue E in the discrete spectrum. (One notes that for the discrete spectrum, the eigenvalues are actually normalizable.) It is then seen that the derivative of E with respect to U_0 is positive. Hence E is increasing with respect to U_0 . A discrete energy is larger than $(2 K_0)$. Increasing U_0 makes it larger, so such

an energy cannot move into the continuous spectrum, as U_0 is increased. This shows that a discrete energy level is not *lost*, when U_0 is increased. However, it could be possible that an additional eigenvalue be moved from the continuous spectrum into the discrete spectrum, as U_0 is increased. So the number of discrete energies is a nondecreasing function of U_0 . The introduction of a new eigenvalue in the discrete spectrum, however, is only possible when there is no gap between the band of continuous spectrum and the possible band of the discrete spectrum. So when U_0 exceeds $(2K_0)$, so that the gap develops, the number of eigenvalues in the discrete spectrum remains constant. The maximum number of the discrete energies is equal to the number of discrete energies for very large U_0 . For $U_0 \rightarrow \infty$, the imaginary part of s_{II} tends to infinity, so that the quantization condition (46) takes the simple form

$$\sin[s_I(n_0 + 1)] = 0, \quad (56)$$

the solutions to which are

$$s_I = \frac{k\pi}{n_0 + 1}, \quad 1 \leq k \leq n_0, \quad (57)$$

where k is in integer. So the maximum number of the discrete energies is n_0 . The eigenvalues corresponding to (57), are of course

$$\frac{E_k}{K_0} = 1 + \frac{U_0}{K_0} - \cos \frac{k\pi}{n_0 + 1}. \quad (58)$$

A similar argument can be used to find values that when U_0 exceeds them a new eigenvalue appears in the discrete spectrum. The argument is that such an eigenvalue should start from the top of the band of continuous spectrum, which is $(2K_0)$, when generation of new discrete eigenvalues are possible. So a new eigenvalue in the discrete spectrum appears as U_0 exceeds a value for which

$$s_{II} = \pi. \quad (59)$$

$$s_I = \cos^{-1} \left(\frac{U_0}{K_0} - 1 \right). \quad (60)$$

For these, the quantization condition (46) becomes

$$\sin[s_I(n_0 + 1)] = -\sin(s_I n_0), \quad (61)$$

which results in

$$s_I = \pi - \frac{(2k - 1)\pi}{2n_0 + 1}, \quad 1 \leq k \leq n_0, \quad (62)$$

where k is integer. The corresponding value for U_0 would be

$$\frac{U_0}{K_0} = 1 - \cos \frac{(2k - 1)\pi}{2n_0 + 1}. \quad (63)$$

In particular, the discrete spectrum is empty if

$$\frac{U_0}{K_0} < 1 - \cos \frac{\pi}{2n_0 + 1}. \quad (64)$$

Of course similar arguments hold for the potential well as well.

3.5 Examples

Consider the potential barrier. The problem is characterized by the dimensionless values (U_0/K_0) , and n_0 . As an example, consider

$$n_0 = 6. \quad (65)$$

The value of (U_0/K_0) determines whether there is a gap between the band corresponding to the discrete energies and the band of continuous energies, or not.

Small barrier. Consider

$$\frac{U_0}{K_0} = 1.5. \quad (66)$$

Here there is no gap between the band of discrete energies, $(E/K_0) \in [2, 3.5]$, and the band of continuous energies, $(E/K_0) \in [0, 2]$. As

$$1 - \cos \frac{7\pi}{13} < 1 - \frac{U_0}{K_0} < 1 - \cos \frac{9\pi}{13}, \quad (67)$$

it is expected from (63) that there are 4 discrete energies. The discrete energies, obtained by the quantization condition (46) and checked by approximate methods, such as the Rayleigh-Ritz perturbation method in the position basis [7], turn out to be

$$\begin{aligned} \frac{E_1}{K_0} &= 2.33248, & \frac{E_2}{K_0} &= 2.76619, \\ \frac{E_3}{K_0} &= 3.14779, & \frac{E_4}{K_0} &= 3.40786. \end{aligned} \quad (68)$$

Large barrier. Consider

$$\frac{U_0}{K_0} = 2.5. \quad (69)$$

Here there is a gap between the band of discrete energies, $(E/K_0) \in [2.5, 4.5]$, and the band of continuous energies, $(E/K_0) \in [0, 2]$. The discrete energies, obtained by the quantization condition (46) and checked by approximate methods, such as the Rayleigh-Ritz perturbation method [7], turn out to be

$$\begin{aligned} \frac{E_1}{K_0} &= 2.60654, & \frac{E_2}{K_0} &= 2.89816, \\ \frac{E_3}{K_0} &= 3.30698, & \frac{E_4}{K_0} &= 3.74878, \\ \frac{E_5}{K_0} &= 4.13895, & \frac{E_6}{K_0} &= 4.40548. \end{aligned} \quad (70)$$

Very large barrier. By this, it is meant that

$$\frac{U_0}{K_0} \gg 1. \quad (71)$$

The discrete energies turn out to be

$$\begin{aligned}\frac{E_1}{K_0} &= 1 + \frac{U_0}{K_0} - 0.90097, & \frac{E_2}{K_0} &= 1 + \frac{U_0}{K_0} - 0.62349, \\ \frac{E_3}{K_0} &= 1 + \frac{U_0}{K_0} - 0.22252, & \frac{E_4}{K_0} &= 1 + \frac{U_0}{K_0} + 0.22252, \\ \frac{E_5}{K_0} &= 1 + \frac{U_0}{K_0} + 0.62349, & \frac{E_6}{K_0} &= 1 + \frac{U_0}{K_0} + 0.90097.\end{aligned}\quad (72)$$

In fact,

$$\frac{E_k}{K_0} = 1 + \frac{U_0}{K_0} - \cos \frac{k\pi}{7}, \quad (73)$$

which is the same as (58).

4 A toy model one-dimensional lattice

In this section, a Kronig-Penney model (on a one-dimensional line) is tailored so that it behaves essentially like a lattice model, to be specific, like something with one single (compact) band for the kinetic energy. The model considered here consists of a particle moving on a line under the influence of a periodic (infinite) array of attractive Dirac delta potentials. It is seen that by adjusting the parameters, one can make the distance between the lowest and the next energy band large, while keeping the position and the width of the band finite, so that essentially there remains only one energy band. This would be like the case of a free particle moving on a one dimensional infinite lattice.

Consider a particle of mass m moving on a line and experiencing a potential energy V , with

$$V(x) = V_r - V_0 \ell \sum_j \delta(x - j\ell), \quad (74)$$

where V_r , V_0 , and ℓ are real constants, V_0 and ℓ being positive. The eigenvalue problem for the Hamiltonian would be

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x) \psi(x) = E \psi(x). \quad (75)$$

The solution to the above in the interval $[-\ell, \ell]$ is represented as

$$\psi(x) = \begin{cases} C \exp(\kappa x) + D \exp(-\kappa x), & -\ell < 0 < x \\ C' \exp(\kappa x) + D' \exp(-\kappa x), & 0 < x < \ell \end{cases} \quad (76)$$

where

$$E = -\frac{\hbar^2 \kappa^2}{2m} + V_r, \quad (77)$$

The continuity conditions at $x = 0$ read

$$C' + D' = C + D. \quad (78)$$

$$\frac{\hbar^2 \kappa}{2m} (C' - D') = \frac{\hbar^2 \kappa}{2m} (C - D) - V_0 \ell (C + D). \quad (79)$$

Also, as the Hamiltonian commutes with translations by the amount ℓ , one can seek eigenvectors of the Hamiltonian which are at the same time eigenvectors of the translation by the amount ℓ (or any integer multiple of that). For such eigenvectors, one has

$$\psi(x + \ell) = \exp(i\alpha) \psi(x), \quad (80)$$

where α is a real constant. (In the terminology of conventional continuum quantum mechanics, such a wave-function ψ is called a Bloch function.) So $\psi(x) \exp(-i\alpha x/\ell)$ is periodic in x with the period ℓ , resulting in

$$C' \exp(\kappa \ell) = C \exp(i\alpha). \quad (81)$$

$$D' \exp(-\kappa \ell) = D \exp(i\alpha). \quad (82)$$

Using these to eliminate C' and D' , and defining

$$\frac{m V_0 \ell^2}{\hbar^2} =: v, \quad (83)$$

$$\kappa \ell =: \beta, \quad (84)$$

by which

$$E = -V_0 \frac{\beta^2}{2v} + V_r, \quad (85)$$

one arrives at

$$\begin{bmatrix} \exp(\beta) & 0 \\ 0 & \exp(-\beta) \end{bmatrix} \begin{bmatrix} 1 - (v/\beta) & -(v/\beta) \\ (v/\beta) & 1 + (v/\beta) \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \exp(i\alpha) \begin{bmatrix} C \\ D \end{bmatrix}. \quad (86)$$

The eigenvalue problem (86) results in

$$\exp(\beta) \left(1 - \frac{v}{\beta}\right) + \exp(-\beta) \left(1 + \frac{v}{\beta}\right) = 2 \cos \alpha, \quad (87)$$

or equivalently

$$\cosh \beta - \frac{v}{\beta} \sinh \beta = \cos \alpha. \quad (88)$$

β could be real or imaginary. (85) shows that the eigenvalues of H which are less than V_r , correspond to real values of β . Obviously, for $v \rightarrow \infty$, the solution of above is $\beta = v$. Based on this, one can develop perturbative solutions for (88). For large values of v one takes

$$\beta = v + \gamma, \quad (89)$$

with $|\gamma| \ll v$, so that

$$\exp(-v) + \left[\frac{\sinh v}{v} - \exp(-v) \right] \gamma + \dots = \cos \alpha. \quad (90)$$

Solving for γ , one arrive at

$$\beta = v [1 + 2 \exp(-v) \cos \alpha + \dots], \quad (91)$$

from which

$$E = -V_0 \frac{v}{2} [1 + 4 \exp(-v) \cos \alpha] + V_r + \dots. \quad (92)$$

So, as $\cos \alpha$ takes values in the interval $[-1, 1]$, the allowed energies form a band of width W , separated by a gap of at least Δ from the next band (the energies larger than V_r , which correspond to imaginary values for β), where

$$W = 4 V_0 v \exp(-v). \quad (93)$$

$$\Delta = V_0 \frac{v}{2}. \quad (94)$$

Clearly,

$$\lim_{v \rightarrow \infty} \frac{W}{\Delta} = 0, \quad (95)$$

meaning that while the width of band can be kept finite, the gap can be set so large that the possible energies are effectively bounded. One can tune V_0 and V_r so that the width of the energy band remains finite and the position of the energy band remains finite as well (as v tends to infinity):

$$V_0 = \frac{W \exp(v)}{4 v}, \quad (96)$$

$$V_r = \frac{W \exp(v)}{8}, \quad (97)$$

for a finite and fixed value of W . With these, in the limit that v tends to infinity, the set of the finite eigenvalues of the Hamiltonian becomes a single energy band. This energy band could be regarded as the values of the kinetic energy for a system on a lattice. One notes that this energy band is actually the sum of a potential energy and a kinetic energy for the original system on the continuum, but the effective spectrum of the total Hamiltonian on the continuum, which is invariant under space translation by the size of the lattice, is the same as the spectrum of kinetic energy of a particle moving on a lattice.

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